

An Evaluation of Temperature Dependent Hall Coefficient of High T_C - Superconductor

AJAY KUMAR SINGH

Department of Physics,
A.M. College, Gaya, Bihar, INDIA.

(Received on: March 19, 2013)

ABSTRACT

Using the theoretical formalism of B. Bucher *et al.* (PRL, 70, 2012) (1993), we have evaluated the temperature dependent Hall Coefficient R_H for high T_C Superconductor $YBa_2Cu_3O_{7-\delta}$ ($T_C = 92K$) for different values of oxygen deficiency δ . Our theoretical results show that R_H increases as a function of temperature and attains maximum value and then decreases. The same behaviour is also observed for others values of δ as $\delta = 0.05, 0.19, 0.23$ and 0.39 . Our theoretically evaluated results are in good agreement with those of the other theoretical workers.

Keywords: Hall coefficient R_H , oxygen deficiency δ , High-temperature superconductor, Mott insulator, antiferromagnetic insulator.

1. INTRODUCTION

It is well known that strong Coulomb repulsion in a narrow band (large μ) can destroy the Fermi-liquid behavior of electron in solids resulting a Mott insulator¹. This is just the case for undoped Copper-based oxides. All of them are antiferromagnetic insulators with magnetic properties satisfactorily described by the anisotropic Heisenberg Hamiltonian contrary to the Fermi-liquid (FL) theory

prediction for a half-filled band. One can expect that while magnetic moments and soft antiferromagnetic fluctuations disappear with doping, high frequency fluctuations (let us say $> 30meV$) survive, giving rise to the spin bipolaron formation proposed by Mott² in accordance with the inelastic neutron scattering experiments by Rossat - Mignod *et al.*³ and by Aeppli *et al.*⁴.

It is now realized that the normal FL can be also destroyed by the strong electron-phonon (Frohlich) interaction.

According to Alexandrov and Ranninger^{5,6} the many electron system on a lattice coupled with phonons turns out to be a charged Bose liquid (BL) consisting on site or inter site small bipolarons (charge $2e$, spin 0 or 1) in the strong-coupling regime.

$$\lambda > \lambda_c \quad (1)$$

with $\lambda_c = 1/\sqrt{2z} < 1$; z is the coordination lattice number. This occurs due to the familiar polaronic collapse of the electron band driven by the boson - vacuum instability. The point is that $\lambda > 1$ is a condition for the polaron formation.⁷ The boson-vacuum instability appears already in the adiabatic description⁸ as in instability of bare phonons at $\lambda = 1/2$: the renormalized phonon frequency $\tilde{\omega} = \omega\sqrt{1-2\lambda}$. The transition for a wide-band electron (or large polaron) to a narrow band small polaron and a small bipolaron is extremely sharp, in the Monte Carlo simulations. Nevertheless the evolution from (1) to charged BL might vary smoothly with the polaronic BCS - like superconductivity in the intermediate coupling region.⁹ The latter has high T_c due to a large density of states in an extremely narrow (less than a thousand K) polaronic band.⁹

The spin bipolarons have some properties which are quite different from those of the lattice bipolarons, for instance, the larger they are, the greater the effective mass. On the other hand, their cooperative properties are those of hard-core charged bosons. In general, both antiferromagnetic and electron-phonon correlations give rise to the polaron and bipolaron formation.

The two microscopic scenarios described above lead to the same ground state (for $\lambda \gg 1$) as the Ogg-Shafroth^{10,11} phenomenological model of preformed local pairs, developed in the last decade by many authors using a negative U Hubbard Hamiltonian.

In this paper, using the theoretical model developed for low energy spin and charge excitation of metal oxides and doped fullerenes, we have studied the temperature dependent Hall coefficient for high T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ ($T_c = 92\text{K}$). We have used different value of δ which gives the oxygen deficiency. In section 2.0, we have presented the mathematical formula used in the evaluation. In section 3.0, we have given the discussion of result. Tables and references are given in the last section of the paper.

2. MATHEMATICAL FORMULA USED IN THE EVALUATION

Now one describes the single model which describe the many features of spinning and charge excitations of the metal oxides. The population of singlet and triplet band is controlled by the chemical potential $\mu = T \ln y$, where y is determined from the thermal equilibrium of singlet and triplet bipolarons.¹² $T > T_c$

$$\ln \left(\frac{1 - ye^{-wT}}{1 - y} \right) + 3 \ln \left(\frac{1 - ye^{(-2w-J)/T}}{1 - y^{-J/T}} \right) = \frac{2nw}{T} \quad (2)$$

and $y = 1$ if $T < T_c$. Here n is the total number of pairs cell and the density of states is

assumed to be energy independent within bands.

Taking the usual contact hyperfine coupling of nuclei with electron spins, one obtains the NMR width due to the spin-flip scattering of triplet bipolarons on nuclei.¹²

$$\frac{1}{T_1} = \frac{AT \sinh(w/T)}{w^2 [\cosh(w/T) - \cosh(w/T)]} \quad (3)$$

with A as a temperature-independent hyperfine coupling constant being of the same order as in simple metals.

The experimentally observed temperature dependence of the integrated absorption intensity.^{13,14}

$$\frac{I(T)}{I(0)} = i_n(T) + i_c(T) \quad (4)$$

where the noncoherent contribution, responsible mainly for the temperature dependence of the normal state absorption, is

$$i_n(T) = 1 - \frac{3BT}{2w} \ln \left(\frac{1 - y \exp(-2w/T - J/T)}{1 - y \exp(-J/T)} \right) \quad (5)$$

and the coherent one :

$$i_c(T) = \delta_c \frac{T^2}{T_c^2} \int_0^{2w/T} x dx \times \left(\frac{1}{y^{-1} \exp(x) - 1} + \frac{3}{y^{-1} \exp(x + J/T) - 1} \right) \quad (6)$$

The temperature independent constant B is proportional to the different of

the noncoherent absorption of singlet and triplet pairs. The triplet half-bandwidth w is assumed to be the same as the singlet one, and the dimensionless constant δ_c determines the relative value of the coherent contribution (i.e., without phonon and spin-wave "shakeoff")

The density of extended (free) bosons is given by (for simplicity we do not distinguish between singlets and triplets).

$$n_b(T) = \frac{T}{2w} - \ln \left(\frac{1 - ye^{-2w/T}}{1 - y} \right) \quad (7)$$

To calculate the density of localized bosons $n_b(T)$ one should take into account the repulsion between them. One can apply a "single well-single particle; approximation assuming that one can place only boson in each potential well due to the Coulomb repulsion between them. Thus, localized charged bosons obey Fermi-Dirac statistics:

$$n_L(T) = \int_{-\infty}^{E_c} \frac{N_L(\epsilon) d\epsilon}{\exp[(\epsilon - \mu)/T] + 1} \quad (8)$$

where the density of localized state $N_L(\epsilon)$ may be approximated in many cases by the exponential tail:

$$n_L(T) = \frac{n_L}{\gamma} \exp \left(\frac{\epsilon - E_c}{\gamma} \right) \quad (9)$$

with γ of the order of the binding energy in a single random potential well and n_L the total number of localized states per unit cell.

The number of empty localized states turns out to be linear as a function of temperature in a wide temperature range $T < (\gamma, 2w)$ because the chemical potential is locked in this temperature region near the mobility edge, which can be chosen equal to zero, $\mu = E_c = 0$. This follows from the conservation of the total number of bosons per cell, $n = n_b(T) + n_L(T)$, which gives for the chemical potential

$$\frac{T}{2w} \ln \frac{1}{1-y} - \frac{n_L(T)}{\gamma} \ln(1+y^{-1}) = n = n_L \quad (10)$$

If $T \ll (\gamma, 2w)$, the solution of this equation is $y \approx 1$ with the exception of a very narrow region of "compensation" $n - n_L \ll T/2w$, where y falls to approximately 0.6 for $\gamma = 2w$. The density, n_b , depends on y logarithmically; therefore, its temperature dependence remains practically linear upto $T \approx \gamma$:

$$n_b(T) = n - n_L + n_L bT \quad (11)$$

with $b = 1/n(1+y^{-1})$ and thus temperature independent.

Solving the Boltzmann equation with a weak magnetic field H for extended bosons, scattered by acoustical phonons, by each other, and by the unscreened random potential, one obtains the expressions for the Hall ratio (R_H), resistivity¹⁵ (ρ), and $\cot \Theta_H$

$$R_H = \frac{v_0}{2e(n - n_L + bn_L T)} \quad (12)$$

$$\rho = \left(m^2 C v_0 / 4e^2 \right) \frac{T + \sigma_b T^2}{n - n_L + bn_L + bn_L T} \quad (13)$$

where $C = C_{av} + n_L C_{im}$ and

$\sigma_b = \alpha e^2 b n_L / m^2 C$ is the relative boson-boson scattering cross-section, and

$$\cot \Theta_H = \frac{cm^2 C}{2eH} (T + \sigma_b T^2) \quad (14)$$

Here v_0 is the volume of an elementary cell (0.167 nm^3 for $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$),

$m = \pi / wa^2$ is the in-plane boson mass, and a is the in-plane lattice constant.¹⁵ The transport relaxation rate due to 2D boson-phonon scattering has been shown to be energy independent and linear in temperature¹² $1/\tau_{b-ac} = mC_{ac}T$, where the constant C_{ac} is proportional to the deformation potential, unoccupied potential wells with the density $bn_L T$ also contribute to the scattering, giving rise the energy-independent elastic relaxation rate, which is linear in temperature:

$1/\tau_{b-im} = mC_{im}n_L T$ with C_{im} as a constant. And, finally, the boson-boson transport relaxation rate has the same temperature dependence as the fermion-fermion scattering and identical to that calculated by Xing and Liu in the case of

localized fermions¹⁶ because the role of the Pauli exclusion principle is played by the dynamical repulsion between localized bosons. This transport relaxation rate is proportional to T^2 because only localized bosons with the energy shell of the order of T near the mobility edge contribute to the scattering and the number of final states is proportional to temperature¹⁶:

$1/\tau_{b-b} = (\alpha e^2 / b n_L / m) T^2$ with α as a constant.

These formulas contain rich information about the number of bosons, localized states, and the relative strength of different scattering channels.¹⁷⁻²⁰

There are two fitting parameters, n and n_L , if no significant variation of $m^2 C$, b and σ_b is expected with doping. Because of the chains the number of in-plane carriers is not fixed by the chemical formula at least in "1-2-3" YBCO.

3. DISCUSSION OF RESULTS

In this paper, we have presented a method of evaluation of temperature dependent Hall coefficient R_H of high T_c superconductor $YBa_2Cu_3O_{7-\delta}$ ($T_c = 92K$) using different values of δ . δ is the oxygen deficiency. We have taken theoretical formalism developed by B. Bucher *et al.*¹⁸ in this evaluation. We have used the formulae given in equation (12) in our evaluation. Our theoretical result indicate that Hall coefficient first increases with temperature attain maximum value at particular temperature and then decreases. The trend is same for all the four values of

$\delta = 0.05, 0.19, 0.23$ and 0.39 . However the magnitude of R_H is large for $\delta = 0.39$. The result is shown in Table T₁. The microscopic parameters used in the evaluation is shown in table T₂. Some recent²¹⁻³⁰ results also show same type of behaviour.

Table T₁

Evaluated result of Hall coefficient R_H as a function of temperature $T(K)$ using formula (12) for high T_c superconductor $YBa_2Cu_3O_{7-\delta}$ ($T_c = 92K$) for different value of oxygen deficiency δ .

T(K)	Hall Coefficient R_H ($10^{-9} \Omega^{-1} m^{-3}$)			
	$\delta = 0.05$	$\delta = 0.19$	$\delta = 0.23$	$\delta = 0.39$
25	0.50	0.45	0.35	0.45
50	0.75	1.45	1.00	1.50
100	1.55	1.56	2.95	3.00
125	1.49	2.25	2.75	3.25
150	1.25	1.95	2.25	3.45
175	1.10	1.75	2.20	3.25
200	0.99	1.49	1.75	2.75
225	0.95	1.49	1.75	2.75
250	0.90	1.45	1.65	2.50
275	0.86	1.26	1.50	2.25
300	0.75	1.00	1.45	2.00
325	0.59	0.95	1.35	1.75
350	0.56	0.75	1.25	1.65

Table T₂Microscopic Parameters of the Model
Determined from the Experimental Data

δ	$n-n_L$	bn_L	m^2C	
		($M10^{-3}K^{-1}$)	($\times 10^{-18}$)	$\sigma_b (\times 10^{-2}K^{-1})$
0.05	0.103	2.22	0.81	1.0
0.19	0.041	1.61	0.69	1.1
0.23	0.035	1.25	0.62	1.2
0.28	0.023	1.11	0.46	1.6
0.39	0.007	0.85	0.46	1.6

ACKNOWLEDGEMENT

I express my sincere thanks to Prof. Lalit Kumar Mishra, Professor, Department of Physics, Magadh University, Bodh Gaya for providing me valuable suggestion and discussion is this paper.

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